

3-Pentenoic acid, 1,1-dimethylethyl ester, (E)-

Inchi:	InChI=1S/C9H16O2/c1-5-6-7-8(10)11-9(2,3)4/h6-7H,5H2,1-4H3/b7-6+
InchiKey:	RMMULFUBQFKFRL-VOTSOKGWSA-N
Formula:	C9H16O2
SMILES:	CCC=CC(=O)OC(C)(C)C
Mol. weight [g/mol]:	156.22
CAS:	81643-03-0

Physical Properties

Property code	Value	Unit	Source
gf	-125.96	kJ/mol	Joback Method
hf	-365.42	kJ/mol	Joback Method
hfus	14.64	kJ/mol	Joback Method
hvap	43.45	kJ/mol	Joback Method
log10ws	-2.42		Crippen Method
logp	2.294		Crippen Method
mcvol	140.810	ml/mol	McGowan Method
pc	2589.85	kPa	Joback Method
tb	482.54	K	Joback Method
tc	675.38	K	Joback Method
tf	260.69	K	Joback Method
vc	0.532	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	308.93	J/molxK	482.54	Joback Method
cpg	371.96	J/molxK	643.24	Joback Method
cpg	360.71	J/molxK	611.10	Joback Method
cpg	348.82	J/molxK	578.96	Joback Method
cpg	336.24	J/molxK	546.82	Joback Method
cpg	322.96	J/molxK	514.68	Joback Method
cpg	382.59	J/molxK	675.38	Joback Method
dvisc	0.0001981	Paxs	482.54	Joback Method
dvisc	0.0002674	Paxs	445.56	Joback Method

dvisc	0.0003809	Paxs	408.59	Joback Method
dvisc	0.0005823	Paxs	371.62	Joback Method
dvisc	0.0009777	Paxs	334.64	Joback Method
dvisc	0.0018672	Paxs	297.67	Joback Method
dvisc	0.0042842	Paxs	260.69	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C81643030&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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